2-Methyl-1-propanol 78-83-1 | DTXSID0021759

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 3.95

Global applicability domain: Inside

Local applicability domain index: 9.78e-01

Confidence level: 8.01e-01

Nearest Neighbors from the Training Set

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2-Methyl-1-propanol Measured: 3.93 Predicted: 3.95 Image not found

2-Butanol

Measured: 3.85 Predicted: 3.95 Image not found

2-Chloroethanol Measured: 4.30 Predicted: 4.07

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tert-Butyl alcohol Measured: 3.50 Predicted: 3.81 Image not found

1-Butanol Measured: 4.19 Predicted: 4.03